

STN

rx

(FILE 'HOME' ENTERED AT 09:43:58 ON 27 AUG 2007).

FILE 'REGISTRY' ENTERED AT 09:44:10 ON 27 AUG 2007

L1 STRUCTURE UPLOADED
L2 0 S L1 EXACT SAM
L3 0 S L1 FAM SAM
L4 1 S L1 SSS SAM

structure p. 46

general to a few structures on p. 46

FILE 'CAPLUS' ENTERED AT 09:45:21 ON 27 AUG 2007

L5 2 S L4

similar for p. 47 str 2

FILE 'REGISTRY' ENTERED AT 09:51:35 ON 27 AUG 2007

L6 STRUCTURE UPLOADED
L7 2 S L6 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:52:17 ON 27 AUG 2007

general to some

structure, on p. 47

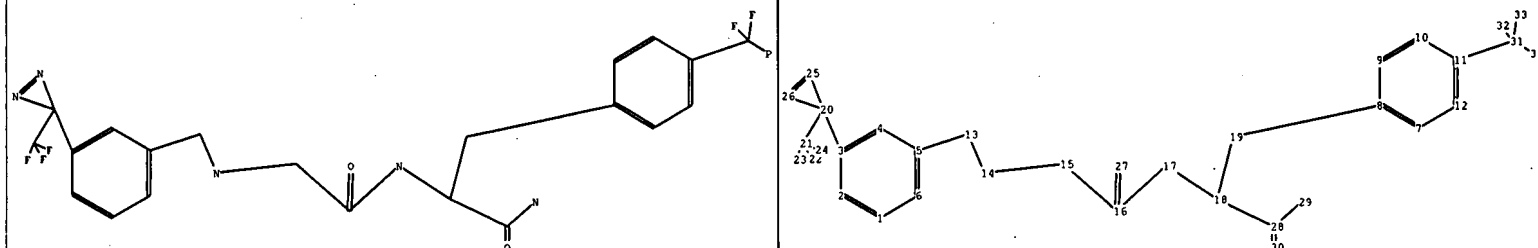
FILE 'REGISTRY' ENTERED AT 09:52:26 ON 27 AUG 2007

L8 22 S L6 SSS FULL

FILE 'CAPLUS' ENTERED AT 09:52:42 ON 27 AUG 2007

L9 3 S L8

e



chain nodes :

13 14 15 16 17 18 19 21 22 23 24 27 28 29 30 31 32 33 34

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 20 25 26

chain bonds :

3-20 5-13 8-19 11-31 13-14 14-15 15-16 16-17 16-27 17-18 18-19
18-28 20-21 21-22 21-23 21-24 28-29 28-30 31-32 31-33 31-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 20-25
20-26 25-26

exact/norm bonds :

13-14 14-15 16-17 16-27 17-18 20-25 20-26 25-26 28-29 28-30

exact bonds :

3-20 5-13 8-19 11-31 15-16 18-19 18-28 20-21 21-22 21-23 21-24
31-32 31-33 31-34

normalized bonds :

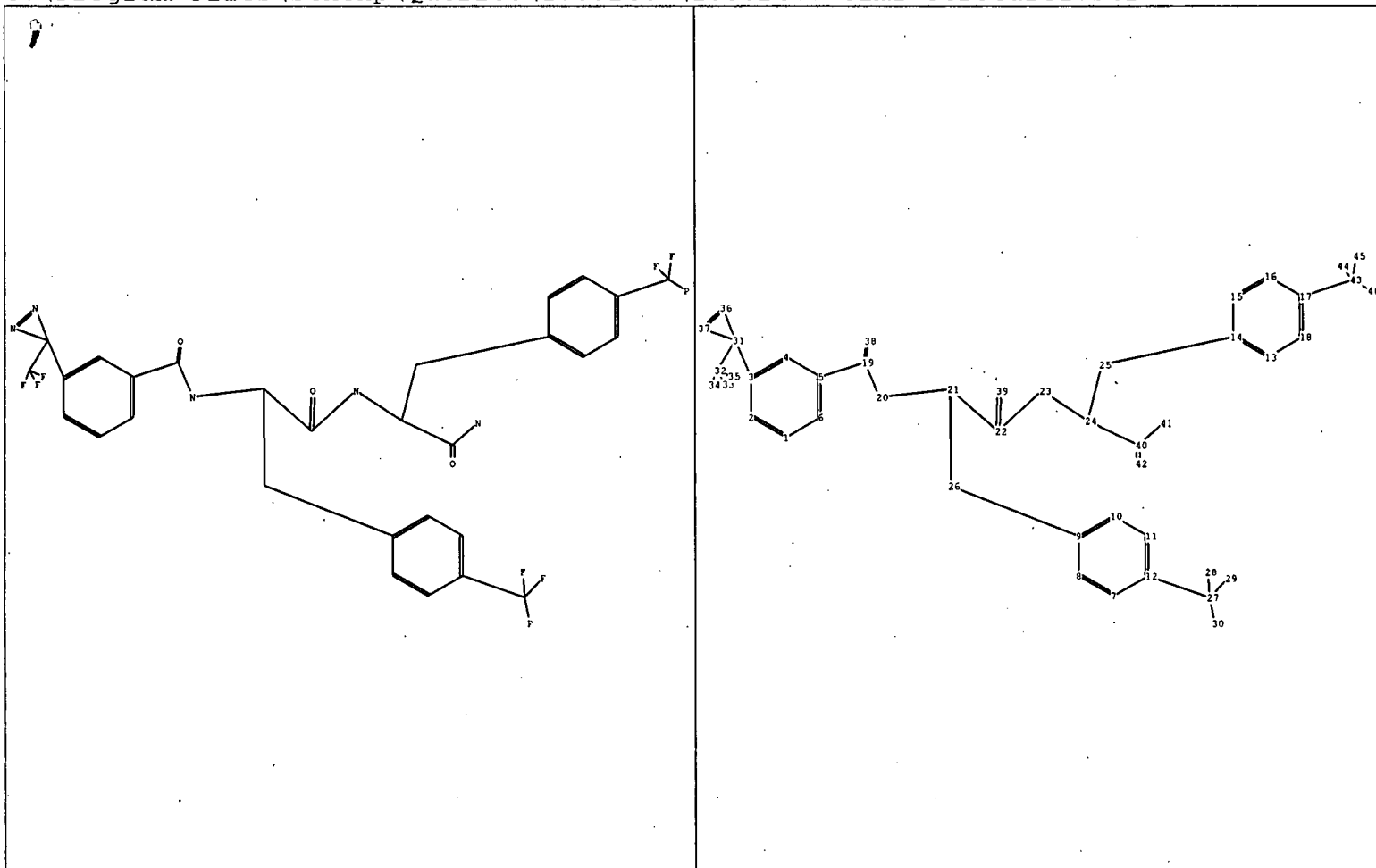
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 19:CLASS 20:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom
26:Atom 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 34:CLASS

STN

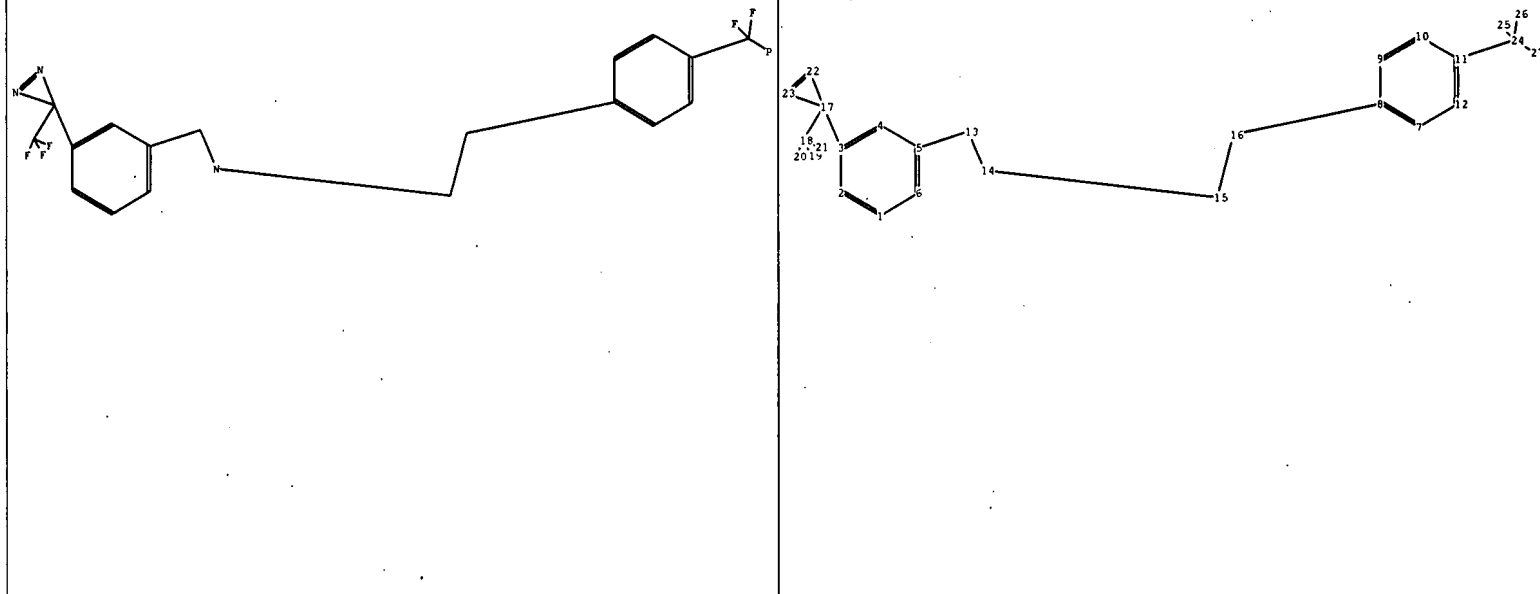
C:\Program Files\Stnexp\Queries\10582467\10582467 clm1 structure1.str



```

chain nodes :
  19 20 21 22 23 24 25 26 27 28 29 30 32 33 34 35 38 39 40
  41 42 43 44 45 46
ring nodes :
  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 31 36 37
chain bonds :
  3-31 5-19 9-26 12-27 14-25 17-43 19-20 19-38 20-21 21-22 21-26
  22-23 22-39 23-24 24-25 24-40 27-28 27-29 27-30 31-32 32-33 32-34
  32-35 40-41 40-42 43-44 43-45 43-46
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14
  13-18 14-15 15-16 16-17 17-18 31-36 31-37 36-37
exact/norm bonds :
  19-20 19-38 20-21 22-23 22-39 23-24 31-36 31-37 36-37 40-41 40-42
exact bonds :
  3-31 5-19 9-26 12-27 14-25 17-43 21-22 21-26 24-25 24-40 27-28
  27-29 27-30 31-32 32-33 32-34 32-35 43-44 43-45 43-46
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14
  13-18 14-15 15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom
32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:Atom 37:Atom 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS
  
```



chain nodes :
 13 14 15 16 18 19 20 21 24 25 26 27
 ring nodes :
 1 2 3 4 5 6 7 8 9 10 11 12 17 22 23
 chain bonds :
 3-17 5-13 8-16 11-24 13-14 14-15 15-16 17-18 18-19 18-20 18-21
 24-25 24-26 24-27
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 17-22
 17-23 22-23
 exact/norm bonds :
 13-14 14-15 17-22 17-23 22-23
 exact bonds :
 3-17 5-13 8-16 11-24 15-16 17-18 18-19 18-20 18-21 24-25 24-26
 24-27
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom
 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom 24:CLASS 25:CLASS
 26:CLASS 27:CLASS